

# Strength of the Vortex-Pinning Interaction from Real-Time Dynamics

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We present an efficient and general method to compute vortex-pinning interactions – as appear in neutron stars, superconductors, and trapped cold atoms – at arbitrary separations using real-time dynamics. This method overcomes uncertainties (associated with matter redistribution by the vortex position and the related choice of ensemble) that plague the typical approach of comparing energy differences between stationary pinned and unpinned configurations: uncertainties that prevent agreement in the literature on the sign and magnitude of the vortex-nucleus interaction. We demonstrate and validate the method with Gross-Pitaevskii-like equations for the unitary Fermi gas, and demonstrate how the technique of adiabatic state preparation with time-dependent simulation can be used to calculate vortex-pinning interactions in fermionic systems such as the vortex-nucleus interaction in the crust of neutron stars.

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Vortex-pinning interactions play an important role in the dynamics of various condensed superfluid systems such as superconductors [1], trapped cold-atom gases [2], and possibly neutron stars [3], where the angular momentum carried by vortices can have an observable impact. Pulsar glitches, for example – sudden increases in the rotation frequencies of neutron stars – are theorized [4] to arise from a sudden macroscopic unpinning of vortices: In equilibrium, the superfluid and non-superfluid components of a pulsar rotate at the same angular frequency. The pulsar loses angular momentum through magnetic radiation, and the crust slows down gradually, reducing the pulsation rate. To maintain equilibrium, the superfluid must also release angular momentum by diluting the vortex concentration, but the presence of pinning sites (nuclei, lattices sites, defects, etc.) may arrest the vortex motion; stress would build until a large number of vortices rapidly unpin, dilute, and transfer their angular momentum to the crust, rapidly increasing in the pulsation rate – the glitch.

Despite almost 40 years, the feasibility of this mechanism is still poorly understood. The conventional picture has the angular momentum stored by the neutron superfluid in the crust (which is well approximated by the same unitary Fermi gas (UFG) produced in cold-atom experiments [5]), with pinning provided by nuclei held in a lattice by the electrostatic (Coulomb) interaction. Recent results suggest that the crustal neutrons may not support enough angular momentum to explain observed pulsar glitches [6], in which case pinning in quark matter phases in the core may play a role [7]. In either case, a reliable technique for calculating vortex-pinning interactions is key. In this paper, we present a dynamical method for determining the sign and strength of vortex-pinning forces in superfluids, and demonstrate that this method can be directly applied to unambiguously calculate the vortex-nucleus interaction using time-dependent density

functional theory (TDDFT) for nuclear matter.

Due to the importance of pinning on glitch phenomenology, several attempts have been made to calculate the pinning force in nuclear matter from underlying microscopic models. The earliest calculations [8] used a Ginzburg-Landau (GL) calculation to estimate the pinning energy as a function of density. In [9] the GL framework was used to give a detailed picture of the pinning/unpinning process: their calculation includes an estimate of the energy as a function of displacement allowing for an estimate of the pinning force. The next advance was the use of a local density approximation [10] with Wigner-Seitz cells and Gogny [11] and Argonne [12] interactions, which gives similar density-dependant pattern of pinning/unpinning as [9], but smaller by almost an order of magnitude.

Unlike vortices in weakly coupled BCS superfluids, vortices in dilute neutron matter (and the UFG) displace a substantial amount of matter from their core [13]. Therefore, comparing “energies” of stationary configurations with a nucleus on the core of a vortex and a nucleus away from the vortex is confounded by a choice of ensemble: should one fix the number of neutrons or the chemical potential in a finite simulation volume?

Computing stationary configurations is also computationally expensive – especially given the high degree of precision required to render meaningful energy differences – and simulations to date have required a high degree of symmetry. For example, recent self-consistent calculations [14–16] extract the binding energy of a vortex on a single nucleus in a cylindrical geometry, which is not the same as the pinning energy. In particular, the conclusion of [15] that the pinning force is repulsive (glitches would thereby requiring interstitial pinning) was questioned by [17], and a different set of calculations using the local density approximation suggests that pinning is attractive over a substantial region in the inner crust [14, 18]. Moreover, nearby vortices and the Casimir effect can sig-

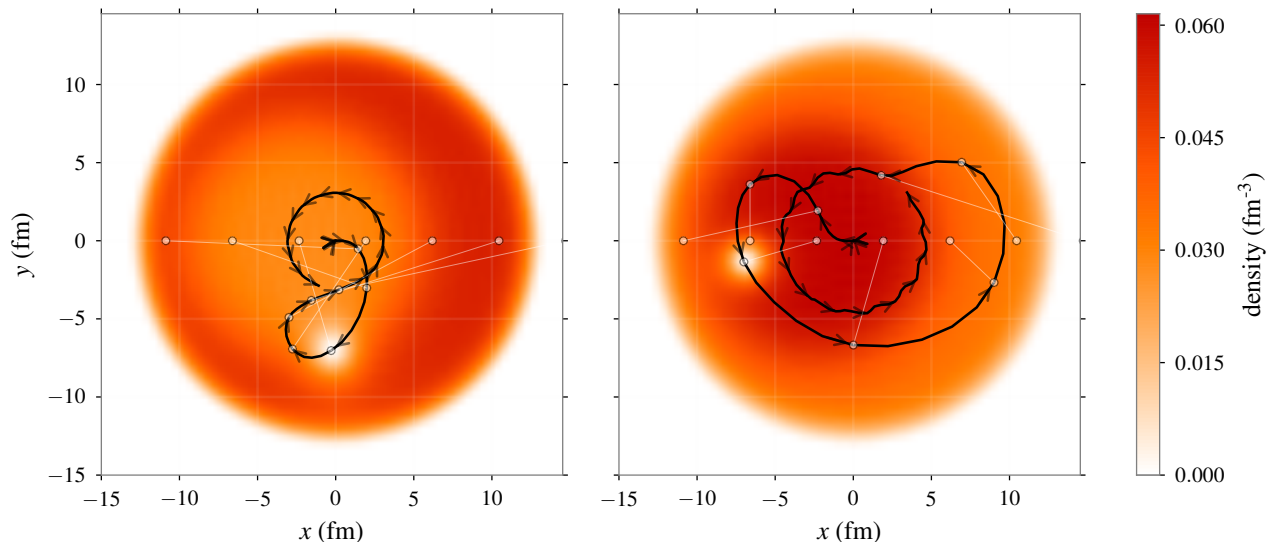


FIG. 1. (Colour online) Deflection of a vortex in the ETF model of trapped dilute neutron matter as a UFG by a repulsive (left panel)/attractive (right panel) pinning potential  $V_{\text{pin}}(r) = \pm 3.5 \text{ MeV}/[1 + \exp(r/\text{fm} - 7.5)]$  moving on a straight line from left to right at a constant subsonic velocity  $v \approx 0.1c_s$ . The trajectory of the vortex is shown by the (black) curve and the relative separation vector between the pinning site and the vortex core is shown as thin (white) lines for select times connecting the corresponding dots on the trajectories. Initially the potential displaces the bulk superfluid, carrying the vortex to the right/left. Once the potential overlaps with the vortex, the vortex rapidly moves down/up – (almost) perpendicular to the force. In the frame shown on the left, the pinning site is just to the left of the centre ( $x \approx -2.5 \text{ fm}$ ) and the vortex is moving (almost) perpendicular along the edge of the pinning potential. After the potential has passed through, the vortex orbits in a counter-clockwise circle direction due to boundary effects from the trap that can be quantitatively described in this sharp, flat trap by placing an image vortex outside of the potential to cancel the tangential current at the boundary: this induces a counter-clockwise super-flow  $v_s$  in Eq. (1). The geometry of the right simulation is such that the potential carries the vortex around almost the entire trap: This extended interaction allows the pinning potential to excite phonons in the system visible as ripples in the circular trajectory.

nificantly polarize a nucleus – an effect absent in simple cylindrical geometries – dramatically changing the nature of the nuclear pinning sites and disrupting the regularity of the nuclear lattice [19].

Characterizing the nuclear-pinning interaction will thus require self-consistent calculations in 3D without symmetry constraints: currently not feasible with techniques that require highly-accurate stationary states, but feasible with TDDFT where the algorithms are substantially more efficient and exhibit better scaling properties. The application of TDDFT for studying fully 3D superfluid dynamic has been demonstrated in [20] and scales well to massively parallel supercomputers. We now present a qualitatively new approach for calculating vortex-pinning interactions, unencumbered by the aforementioned issues, and utilizing only real-time dynamics.

The idea, similar to the Stern-Gerlach experiment, is to observe how a vortex moves when approached by a nucleus. To zeroth order, the sign of the interaction is determined qualitatively by the direction of the motion (Fig. 1); with a more careful inspection, one can extract the force-separation relationship  $F(r)$  (Fig. 2).

We validate our procedure using a dynamical extended Thomas-Fermi (ETF) model [21–24], equivalent to a

Gross-Pitaevskii equation (GPE) for bosonic “dimers”  $m_B = 2m$  of fermionic pairs, with an equation of state tuned to consistently fit both quantum Monte Carlo (QMC) and experimental results [23]. Despite the computational simplicity of the ETF model, it has been demonstrated to quantitatively reproduce low-energy dynamics of both UFG experiments [22] and fermionic density functional theory (DFT) simulations [24]; in the latter case, the ETF also characterizes numerical effects such as finite size and discretization artifacts. The UFG should also qualitatively model the dilute neutron superfluid in the crust of neutron stars [25] due to the large neutron-neutron scattering length  $a_{nn} \approx -18.9 \text{ fm}$  [26]. Thus, by using a physically motivated model of the nuclear pairing potential [11], we anticipate these ETF calculations to faithfully simulate future fermionic TDDFT simulations.

To gain some intuition for the vortex-nucleus interaction, consider the phenomenological Hall-Vinen-Iordanskii (HVI) equation (see [27] for a discussion) for a vortex in 2D:

$$M\ddot{\vec{r}}_v - \vec{f}_{qp} = \rho_s \vec{\kappa} \times (\dot{\vec{r}}_v - \vec{v}_s) + \vec{F}_v. \quad (1)$$

Here  $\vec{r}_v$  is the position of the vortex, the force  $\vec{F}_v$  is per unit length along the vortex,  $\rho_s$  is the number density of

the “background” superfluid,  $\vec{\kappa} = 2\pi\hbar\hat{z}$  is the quantized vortex circulation, and  $\vec{v}_s$  is the “background” superfluid velocity. This equation should only be taken as an intuitive guide since terms on the left-hand side are ill-defined. The “mass of the vortex”  $M$ , for example, depends strongly on the way it is measured [28], and the force  $\vec{f}_{qp}$  due to excited phonons has significant memory effects.

One can argue that the left side of this equation is of higher order than the right side for small velocities of the pinning site, and, as we shall verify in Fig. 2, can be neglected for the application of vortices in neutron stars where the pinning force is quite weak and moves slowly. This leaves the well-established Magnus relationship  $\rho_s \vec{\kappa} \times (\vec{r}_v - \vec{v}_s) \approx -\vec{F}_v$  relating the force  $\vec{F}_v$  applied to the vortex and its perpendicular velocity  $\dot{\vec{r}}_v$  relative to the background superfluid velocity  $\vec{v}_s$ . Thus, by observing the dynamical deflection of a vortex from a nuclear pinning site, one can directly extract the direction and approximate magnitude of the vortex-nucleus force without requiring a subtle subtraction of energies.

In small systems, the Magnus relation can only be used to estimate the magnitude of the force since the superfluid density  $\rho_s$  and velocity  $v_s$  are not precisely defined, though reasonable estimates can be obtained. With an external pinning potential  $V_{\text{pin}}(\vec{r}_{\text{pin}} - \vec{x})$ , however, one can directly and unambiguously calculate the force on the pinning site:


$$\vec{F}_{\text{pin}} = - \int d^3x \frac{\partial V_{\text{pin}}(\vec{r}_{\text{pin}} - \vec{x})}{\partial \vec{r}_{\text{pin}}} \rho(\vec{x}). \quad (2)$$

In the nuclear context where neutrons are present in the both the pinning site (the nucleus) and the superfluid medium, the force can be obtained in two ways: 1) Eq. (2) can be directly applied to a Coulomb potential that traps the protons – this will be the force that the vortex exerts on the nuclear lattice – or, 2) one can estimate the force using Newton’s law  $\vec{F}_{\text{pin}} = m_{\text{pin}} \vec{a}_{\text{pin}}$  for a dynamic pinning site comprising protons and entrained neutrons. The position of the pinning site can be unambiguously defined as the center of mass (CM) of the protons, and the effective mass  $m_{\text{pin}}$  can be estimated limiting forms in homogeneous matter [29].

What remains is to prepare the initial conditions with a vortex and nucleus interacting at various distances. We can do this using adiabatic state preparation [30], thereby eschewing the need for diagonalizing large matrices to find stationary initial conditions. The idea is to adiabatically evolve in real-time a state of some solvable system to a desired initial state in the system of interest. For example, starting with a non-interacting harmonically trapped gas, we can evolve either the ground state  $\Psi_{GS} \propto \exp(-m_B \omega r^2 / 2\hbar)$ , or an exact “Landau level”  $\Psi_\delta \propto (x + iy - \delta) \exp(-m_B \omega r^2 / 2\hbar)$  (stationary in a rotating frame) with angular momentum  $l_z = N\hbar / (1 + m\omega\delta^2/\hbar)$ . We adiabatically evolve the system while turning on the interactions  $s\xi$  and adjusting

the trapping potential  $V_t = (1 - s)V_{HO} + sV_{\text{trap}}$  with a  $C^\infty$  function  $s(t/T) = \text{—}$  that goes from 0 to 1 over a characteristic time  $T$  chosen to be longer than any intrinsic timescale in the system:

$$s\left(\frac{t}{T}\right) = \frac{1}{2} + \frac{1}{2} \tanh \left[ \alpha \tan \left( \frac{\pi t}{T} - \frac{\pi}{2} \right) \right] = \text{—} \quad (3)$$

(The parameter  $\alpha$  controls the smoothness and we find empirically that values  $1 < \alpha \lesssim 6$ :  work well.) From  $\Psi_{GS}$  we can generate the ground state, and from  $\Psi_{\delta=0}$  we can generate a single vortex in the centre of the trap, both to high precision. Producing a state  $\Psi_\delta$  with a single orbiting vortex off-axis vortex proves to be more challenging – one often finds incommensurate “phonon sloshing” in addition to an orbiting vortex (similar to the final state in the right of Fig. 1).

To accurately measure the vortex-pinning interaction one can choose as a final potential  $V_T = V_{\text{trap}} + V_{\text{pin}}$ : an axially symmetric trap of suitably flat bottom and a pinning potential in the center. By generating a configuration with a vortex orbiting in a circle at radius  $r$ , we can use Eq. (2) to calculate the force exerted on the centrally located pinning potential: axial symmetry ensures that this is precisely the vortex-pinning force at separation  $r$ . We use this procedure within the ETF model to accurately calculate the “stationary” (in a rotating frame) vortex-pinning interaction shown in Fig. 2.

This procedure is not ideal with the adiabatic state preparation due to the sloshing. Instead, one can prepare a central vortex  $\Psi_{\delta=0}$ , and then directly probe the force using a “dynamic” simulation as shown in Fig. 1 for a large range of interaction. (The perpendicular motion of the vortex makes it somewhat difficult to probe very short-range interactions with this approach.) The feasibility of this approach is verified in Fig. 2 where we directly compare it with the vortex-pinning interaction extracted by the stationary method.

The present demonstration has been limited to quasi-2D simulations. The procedure will work just as well in fully 3D simulations. New effects such as the bending of a vortex line when approached by a pinning site can just as easily be analyzed: the vortex line will either be repelled by the pinning site – bowing out to avoid it – or will be sucked in. Again, qualitative dynamical behaviour coupled with the techniques demonstrated here can be used to extract the 3D characteristics of the vortex-pinning interaction. We have considered here only moving the pinning site, but one could also consider manipulating parts of the vortex with pinning potentials, dragging the pinned vortex along a trajectory instead. In simulations with realistic nuclei, the vortex-nucleus interaction will also excite and deform the nucleus – significantly affecting the vortex-nucleus interaction. It is conceivable also that a vortex lines could break and attach to various nuclear defects like rods of plates: the dynamics of such broken

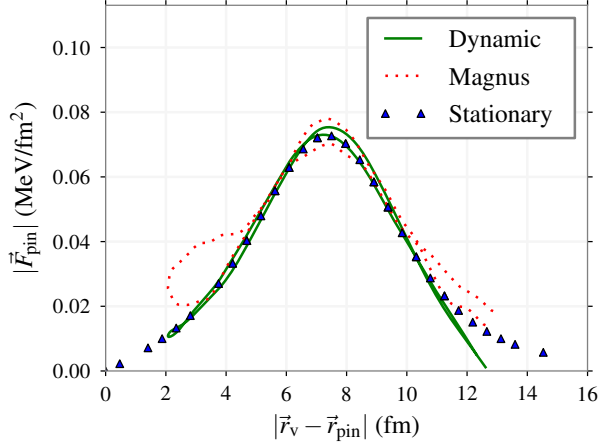


FIG. 2. (color online) Here we demonstrate the consistency of dynamically extracting the vortex-pinning force for the nuclear pairing potential [11]  $V_{\text{pin}}(r) = 0.75 \text{ MeV}/[1 + \exp(r/\text{fm} - 7.5)]$  at densities  $\rho \sim 0.045 \text{ fm}^{-3} \approx 0.28\rho_{\text{sat}}$ . The triangular (blue) points come from the computationally expensive “stationary” method, while the solid (green) curve come from using the “dynamic” real-time evolution analogous to that shown on the left panel of Fig. 1. The dotted (red) curve shows the Magnus estimate for the force (1) using a Thomas-Fermi approximation for  $\rho_s$  and estimating  $\vec{v}_s$  from the image vortex [31]. The double curves represent the interaction as measured from the incoming and outgoing pinning site.

vortex lines may also play a important part in explaining neutron star glitches.

We close with a brief analysis of the time-evolution. The complex scalar field  $\Psi$  obeys an evolution equation of the form

$$i\hbar\dot{\Psi} = \left( -\frac{\hbar^2\vec{\nabla}^2}{2m_B} + V_{\text{eff}}[\Psi] \right) \Psi \quad (4)$$

where  $V_{\text{eff}}[\Psi]$  is an effective interaction that depends nonlinearly on  $|\Psi|$  and on the external trapping and pinning potentials. Consider the quasi-two-dimensional problem where coordinates may be expressed as complex numbers  $z = x + iy$ : A singly-wound vortex at location  $z_v$  may be described by the field  $\Psi(z) = (z - z_v)f(z)$ , where  $f(z)$  is a smooth complex-valued function that we assume has no roots in the immediate vicinity of the vortex. The evolution equations may then be expressed as follows

$$\begin{aligned} i\hbar\dot{f} + \frac{\hbar^2\vec{\nabla}^2 f}{2m_B} - V_{\text{eff}}[\Psi]f \\ = \frac{i\hbar\dot{z}_v f - \hbar^2(\partial_x f + i\partial_y f)/m_B}{z - z_v}. \end{aligned} \quad (5)$$

The left side is smooth, hence the pole on the right side must cancel with a root in the numerator, giving us an

explicit expression for the vortex velocity

$$\dot{z}_v = [\dot{r}_v]_x + i[\dot{r}_v]_y = \hbar \frac{-i\partial_x f + \partial_y f}{m_B f} \Big|_{z=z_v}. \quad (6)$$

This expression can be written as the “Magnus” relation

$$\vec{\kappa} \times (\dot{\vec{r}}_v - \vec{v}) = \frac{\hbar^2 \vec{\nabla} \rho}{2m_B \rho} \Big|_{z=z_v} \quad (7)$$

where the local “superfluid velocity”  $\vec{v}$  is

$$f = \sqrt{\rho} e^{i\phi}, \quad \vec{v} = \vec{\nabla} \phi. \quad (8)$$

Note that the relationship (7) is exact. The meaning of  $\rho_s$  in the HVI equations is not clarified since  $\rho$  cancels in (7). Unfortunately, although  $\vec{v}$  is precisely defined and corresponds to  $\vec{v}_s$  in some situations, one cannot generally make the correspondence  $\vec{v}_s \equiv \vec{v}$ . In particular, doing so yields results that differ by as much as 50% in Fig. 2.

The quantities appearing in Eq. (1) are related to long-range momentum transfers and boundary effects, and one must thus be content with reasonable estimates for  $\rho_s$  and  $v_s$ , for example, from the average behaviours of the relevant quantities near but outside of the vortex core. As Fig. 2 demonstrates, however, the Magnus relation is suitable for extracting the sign and magnitude of the interaction. This also provides an explicit check that the force evaluated using our procedure is what appears on the right side in Eq. (1) governing the vortex dynamics.

*Conclusion:* We have described how to use time-dependent density functional theory (TDDFT) to efficiently and unambiguously calculate vortex-pinning interactions from real-time dynamical simulations of superfluid systems. We have demonstrated with an extended Thomas-Fermi (ETF) model of the unitary Fermi gas (UFG) that this approach can be applied to calculate the vortex-nucleus interaction using nuclear TDDFTs to model the crust of neutron stars. While we considered only quasi-2D systems here, the size of the problem, the magnitude and accuracy of the force extraction, and the use of pure real-time dynamics ensure that full 3D simulations of realistic fermionic TDDFTs will be within the capabilities of next generation supercomputers. A resolution to the puzzle of pulsar glitches will requiring more than just extracting the vortex-nucleus interaction, but with this real-time method, this crucial step will soon be within reach.

These techniques can also be directly applied to systems of trapped ultra-cold atoms in a variety of geometries, for example, to explore vortex pinning on optical lattices. In particular, the close approximation of the neutron superfluid by the UFG suggests that cold atom experiments might also be able to shed light on the glitching puzzle.

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